Nucleation of bended vortices in Bose-Einstein condensates in elongated traps.

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We study the generation of vortices in rotating axially elongated magneto-optical traps, a situation which has been realized in a recent experiment (K. W. Madison, F. Chevy, W. Wohlleben, J. Dalibard, Phys. Rev. Lett. **84** 806 (2000)). We predict that at a critical frequency the condensate experiences a symmetry breaking and changes from a convex cloud to a state with one bended vortex. We also discuss several effects which enlarge the critical frequency with respect to other geometries of the trap: these are, (i) the failure of the Thomas-Fermi approximation on the transverse degrees of freedom of the condensate, (ii) the enhancement of the transverse asymmetry of the trap by means of rotation and (iii) the yet unobserved bending of the vortex lines.

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Since the creation of the first Bose-Einstein condensates (BEC) using ultracold dilute gases [1] and the success in describing them using simple but accurate mean field theories, it has been a goal of the field to produce and understand the Physics behind vortices in these condensates.

Vortices, or vortex-lines we should rather say, constitute the most relevant topological defect that one finds in Physics. They basically consist on a twist of the phase of a wave function around an open line and they are typically associated to a rotation of a fluid whatever the fluid is made of (real fluids, optical fluids, quantum fluids, ...) [2]. Furthermore, vortices are one of the means by which quantum systems may acquire angular momentum and thus react to some perturbations of the environment. They have already been predicted, observed and studied in the superfluid phase of ^{4}He and are indeed known to be the key to some important processes inside these systems, such as dissipation, moments of inertia and breakdown of superfluidity. This is why extensive research on vortex generation, stability and dynamics has been conducted in the field of BEC in the last years [3–6].

In a recent experiment performed by a group from the École Normale Supérieure (ENS) [7] vortices are created by rotating an elongated trap slightly deformed in the trasverse dimensions. This rotation is performed at a constant angular speed, Ω, which is the key parameter for the appearance of one or more vortices. Many interesting phenomena have been observed in these experiments, but we are concerned with some of them which are controversial: (i) the first vortex nucleates at a critical rotation speed or *critical frequency*, Ω_1, larger than the estimate of $\Omega_1^{TF} = \frac{5\hbar}{2mR_\perp^2} \ln \frac{0.671 R_\perp}{\xi}$ [8], (ii) vortex cores seem partially filled and (iii) after the nucleation of the first vortex the angular momentum seems to depend continuously on the rotation speed.

In this letter we consider these effects within the framework of a mean field theory for dilute gaseous condensates

in rotating traps. In addition to an explanation of the experimental features we find the surprising fact that above Ω_1 a symmetry breaking changes the ground state (GS) into a *bended* vortex [Fig. 1]. We will discuss this phenomenon later.
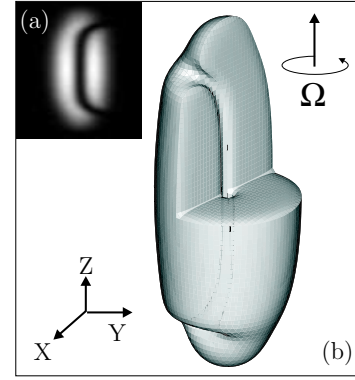

FIG. 1.   Shape of the ground state of the Hamiltonian (3) for $\Omega = 0.75\omega_\perp, \gamma = 350, Ng = 1000$ and $\varepsilon = 0$. (a) Trasverse section. (b) Density plot. One quarter of the condensate has been removed to allow the direct observation of the inner structure of the vortex line.

The model.- For most of the current experiments it is an accurate approximation to use a zero temperature many-body theory of the condensate. In that limit the whole condensate is described by a single wavefunction $\psi(\mathbf{r}, t)$ ruled out by a Gross-Pitaevskii equation (GPE).

In the ENS experiment the trap is initially harmonic with axial symmetry, but then a laser is applied which deforms it and makes it rotate with uniform angular speed Ω. By using the mobile reference frame which rotates with the trap, we can describe this experiment using a modified GPE which reads

$$i\frac{\partial \psi}{\partial t} = \left[-\frac{1}{2}\triangle + V_0(\mathbf{r}) + g\left|\psi\right|^2 - \Omega L_z \right] \psi. \qquad (1)$$

Here the ENS trapping potential is given by

$$V_0(\mathbf{r}) = \frac{1}{2}\omega_\perp^2(1-\varepsilon)x^2 + \frac{1}{2}\omega_\perp^2(1+\varepsilon)y^2 + \frac{1}{2}\omega_z^2 z^2. \quad (2)$$

and $L_z = i\,(x\partial_y - y\partial_x)$ is a linear operator which represents the angular momentum along the z-axis.

In Eq. (1) we have already applied a convenient adimensionalization which uses the harmonic oscillator length, $a_\perp = \sqrt{\hbar/m_{Rb}\omega_\perp}$ and period, $\tau = \omega_\perp^{-1}$. Using these units the nonlinear parameter becomes $g = a_S/a_\perp$, where $a_S \simeq 5.5\,\text{nm}$ is the scattering length for ^{87}Rb, which is the gas used in Ref. [7]. Following the experiment we will take $\omega_z = 2\pi \times 11.6\,\text{Hz}$ and $\omega_\perp = 2\pi \times 232\,\text{Hz}$. Through the paper we will also use a fixed value of $Ng = 1000$ which corresponds to a few times 10^5 atoms. For the small transverse deformation of the trap we have used $\varepsilon = 0.03, 0.06, 0.09$ ($\varepsilon = 0.03$ is the closest one to the actual experiment).

The norm, $N[\psi] = \int |\psi|^2\,d\mathbf{r}$, which can be interpreted as the number of bosons in the condensate is a conserved quantity as well as the energy

$$E[\psi] = \int \bar\psi\left[-\frac{1}{2}\triangle + V_0\,(\mathbf{r}) + \frac{g}{2}\,|\psi|^2 - \Omega L_z\right]\psi d\mathbf{r}. \quad (3)$$

Each stationary solution of the GPE of the form $\psi_\mu(\mathbf{r},t) = e^{-i\mu t}\phi(\mathbf{r})$, is a critical point of the energy subject to the constraint of the norm, $\left.\frac{\partial E}{\partial \psi}\right|_N [\psi_\mu] = 0$.

Ground states.- It is physically plausible to assume that the ENS experiment actually produces condensates which are close to the *absolute minimum of the energy* subject to some constraints. In practice, this means that any theoretical effort to reproduce the experimental results must be based on a method to find these *ground states* of Eq. (3) for given norm and rotation speed. To achieve this goal and to be able to make quantitative predictions we have worked numerically with the energy functional [Eq. (3)], using a method known as Sobolev gradients. This method is a preconditioned descent technique which allows to get accurate approximations to the ground state where other minimization procedures fail. We have applied this method over a Fourier basis with $32 \times 32 \times 64$ modes, which is enough to obtain accurate estimates of macroscopic values, such as the angular momentum and the lowest critical frequencies. Nevertheless, the most controversial results have been confirmed on a grid with $64 \times 64 \times 128$ modes.

Our simulations are summarized in Figs. 1 and 2. The first striking prediction is that vortex lines are nucleated with a deformed shape, like a tight string which is pulled from the middle as rotation is increased [Fig. 1]. The second important result [Fig. 2(b),(d)] is that even for a weak trap anisotropy, $\varepsilon = 0.1$ [Fig. 2(d)] a transverse section of the condensate shows a very deformed cloud: the rotating condensate amplifies the small transverse deformation which is used to transfer angular momentum to the condensate.

Furthermore, Fig. 2 reveals that our numerical simulations confirm several other features already found in the experiment. First, the critical frequency for the nucleation of a vortex Ω_1 is larger than what it is expected in the spherically symmetric trap. According to Fig. 2(a) in our simulations (see parameters above) the condensate remains in a vortexless state until $\Omega = 0.7(1) \times \omega_\perp/2\pi$, that is, $\Omega_1 \simeq 162$ Hz, which is close to the value of 147 Hz obtained experimentally [7], but far from the Thomas-Fermi estimate for radially symmetric clouds.
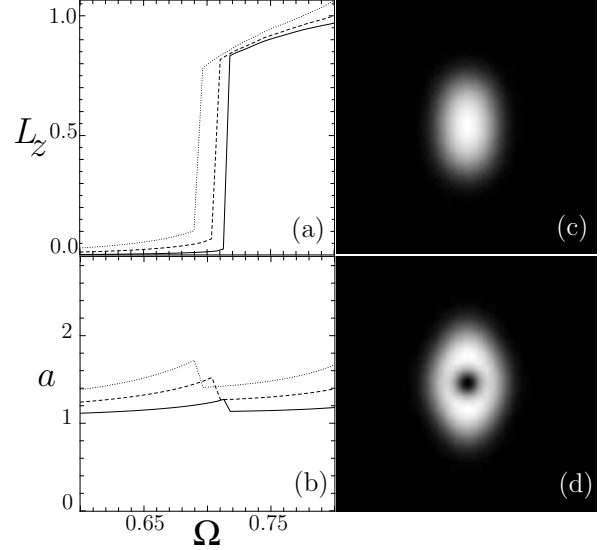

FIG. 2. (a-b) Angular momentum, L_z, and shape factor, $a = \langle y^2\rangle/\langle x^2\rangle$, of the GS of $E(\psi)$ [Eq. (3)] as a function of Ω. Solid, dashed and dotted lines correspond to $\varepsilon = 0.03, 0.06, 0.09$ respectively. (c-d) Transverse density plots of a GS without vortex ($\Omega = 0.65, \varepsilon = 0.1$) and a GS with one vortex ($\Omega = 0.75, \varepsilon = 0.1$). Pictures are 12×12 adimensional units large.

The second remarkable feature is that, at $\Omega = \Omega_1$ the angular momentum per particle $\langle L_z\rangle/N$ jumps to a value which is smaller than 1 and which grows continuously until a second vortex is nucleated [Fig. 2(a)].

Thus, the numerical simulations are in good agreement with the experience and both contradict previous ideas: (i) the nucleation frequency is much larger than expected in Thomas-Fermi theories, and (ii) the angular momentum has a continuous, nonlinear dependence on Ω. To obtain more insight on the physical reasons for this behaviors we will analyze several simplified situations.

Critical frequencies for axially symmetric traps .- Let us first consider the case of an axially symmetric trap. For these traps it is usually thought that at a certain $\Omega = \Omega_1$ the system experiences a transition from a vortexless state to a *symmetric* state with one vortex. Both states do also exist in the nonrotating case and have energies E_0 and $E_1 > E_0$, respectively. This leads to the usual estimate of the critical frequency $\Omega_1 \simeq E_1 - E_0$.
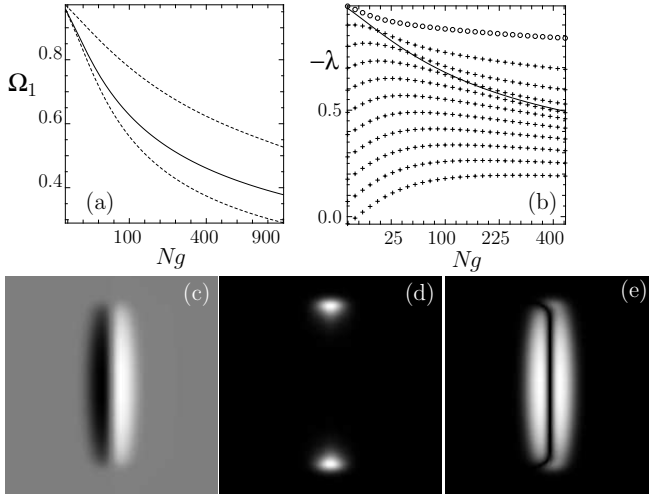
FIG. 3. (a) Critical frequency, Ω_1 for a spherical trap ($\gamma = \omega_\perp^2/\omega_z^2 = 1$, solid line), a cigar shape trap ($\gamma = 19$, upper dashed line) and a pancake trap ($\gamma = 1/19$, lower dashed line). (b) Critical frequency Ω_1 (solid line) and eigenvalues arising from the linearization of the energy (circles) for a trap with $\gamma = 19$. It is remarkable that there is always a negative eigenvalue which is not suppressed for $\Omega = \Omega_1$. (c) Vortex, (d) main destabilizing mode and (e) bended vortex line arising from a combination of both, for a trap with $\gamma = 19$.

Taking the previous idea for granted and to learn how the *elongation of the trap* affects the nucleation of the first vortex, we have searched the vortexless state and the state with one vortex in different *axially symmetric* traps ($\varepsilon = 0$), computing $\{E_0, E_1, \Omega_1\}$. The result of these calculations is shown in Fig. 3(a) for different elongations. There we see that the critical angular speed of a cigar shape trap is larger than that of spherically symmetric and pancake traps. The explanation is simple: in an elongated trap, $\omega_z \ll \omega_\perp$, the system expands preferably along the axial dimension in order to accommodate more bosons and counteract the interaction energy. As ω_z is made smaller this tendency becomes more evident, since the transverse shape no longer satisfies the Thomas-Fermi approximation in which the second order derivatives are negligible. Instead, the transverse shape of the cloud is closer to a harmonic oscillator wavefunction, and as such the energy required to introduce a single vortex, Ω_1, becomes larger than in the spherically symmetric case. In other words, the more elongated the trap is, the more dilute the condensate seems on the XY plane, the closer Ω_1 becomes to its linear limit $\omega_\perp$, and the faster the condensate must spin to accept a vortex. This effect, which can be characterized as a dynamical separation of longitudinal and transverse degrees of freedom [9], manifests in a departure of Ω_1 from any Thomas-Fermi based results, which correspond to a regime ruled by the transverse self-interaction of the condensate.

Bended vortices in axially symmetric traps.- An important feature of elongated traps is that they require very

little energy to produce longitudinal excitations of the condensate [5]. This makes feasible for small perturbations to induce longitudinal modes and distortions of the vortex lines [10,12]. Thus our next step is to perform a linear stability analysis of the straight vortex line which we have already found.

We are looking for a quadratic expansion of the energy of a perturbed vortex. Since the vortex ψ_{vort} is a stationary state, this energy must read, up to second order perturbations

$$E(\psi_{vort} + \epsilon\delta) \simeq E_1 - \Omega + \epsilon^2 \sum_i (\lambda_{i,m} - m\Omega) |c_{i,m}|^2 \quad (4)$$

Here, $\lambda_{i,m}$ are the different eigenvalues which arise from linearizing the GPE [Eq. (1)] around ψ_{vort}, m are their vorticities with respect to ψ_{vort} (See [5]), and $c_{i,m}$ is the weight of the $|i, m\rangle$ mode in the expansion of $\delta(\mathbf{r})$. By finding the lowest negative eigenvalue, $\lambda_{i,-1} < 0$, we know that at a rotation speed $\Omega_{meta} = |\lambda_{i,-1}|$ the energy (4) becomes positive for all perturbations and the vortex is locally stable or *metastable*.

These calculations are summarized in Fig. 3(b). There we plot all eigenvalues $-\lambda_{i,-1}$ and find that there is a number of them such that $-\lambda > (E_1 - E_0)$. This result suggests that there exists a range of speeds $\Omega \in (\Omega_1 = E_1 - E_0, \Omega_m)$ in which the system nucleates a vortex, but that vortex does not have a symmetric shape. Instead, the stability analysis points out that this vortex is bended by its ends, forming a curved vortex line [Fig. 3(e)]. Although this is a perturbative prediction arising from the linear stability analysis, these solutions are consistent to what we formerly obtained by minimizing the full Hamiltonian and which was explained above [Fig. 1].

The existence of a ground state with such a bended shape is one of the main predictions of the paper, since it presents a symmetry breaking due solely to rotation. In some sense the symmetry is broken twice: First because a phase asymmetric structure, the vortex, appears, and a second time because the vortex bends in some specific direction. We have also observed that as the frequency is increased from Ω_1 the vortex bending becomes less and less evident (And $\langle L_z \rangle$ approaches N). However, when the threshold Ω_2 for the nucleation of two vortices is reached the bending becomes again very important.

The existence of bending in the vortex lines may be checked in the experiment and is probably related to the experimental observation that vortex lines appear to be partially filled when viewed from above.

Role of transverse asymmetries.- In Ref. [7] the trap is distorted over the transverse directions to induce some mechanical response of the condensate, an effect which must be taken into account.

As it was already shown [11] any initial asymmetry of a condensate is strongly emphasized by the rotation of the trap, an effect that may be estimated analytically in the

linear and Thomas-Fermi limits. These estimates lead to a value of the angular momentum for a vortexless condensate and a different one for a condensate with a single, centered, unit-charge vortex line. The main difference with respect to the symmetric case is that a vortexless state may acquire some angular momentum and that the nucleation of a vortex line gives an increase of the total angular momentum which is inversely proportional to the asymmetry factor, ε. From a practical point of view this means that the system may "decide" to wait for a larger rotation speed $\Omega_1 > \Omega_{1,sym}$ before nucleating a vortex. Actually what happens is that $\Omega_1/\min(\omega_x, \omega_y)$ increases with respect to ε, but $\Omega_1/\omega_\perp$ decreases [Fig. 2].

Although it is clear that the effect of transverse asymmetries is to provide a larger critical frequency than expected it is not possible to use any analytic estimate of the critical speeds because of the elongation of the trap and its transverse deformation. Furthermore, due to the bending of the vortex lines it is not possible to work with the corrections from [11] to get a reliable estimate of Ω_1.

Discussion and conclusions.- We have used the GPE to study theoretically the nucleation of vortices in an elongated trap similar to that of the ENS experiment [7]. We have found several mechanisms which lead to an increase of the angular speed which is required to create those vortices and have found the remarkable feature that vortex lines are bended by their ends. This provides some kind of symmetry breaking bifurcation in the case of a single vortex [13]. Recalling previous experience with liquid helium, we suspect that this bending has some important consequences, and that it might be responsible for the breakdown of superfluidity in BEC by a mechanism which consists in several vortex lines joining together and forming a turbulent pattern.

Using only the special geometry of the experiment we have obtained a value of $\Omega_1 = 0.7(0)\omega_\perp$ which is close but above the experimental value. However, this means that the experiment implies a systematic negative shift both in Ω_1 and in the angular speed at which the superfluid escapes, Ω_c. In the experiment $\Omega_c \simeq 2\pi \times 210$ Hz, while the theory predicts $\Omega_c = \omega_\perp(1 - \varepsilon)$. If we trust the value of Ω_c from the experiments Ω_c and make $\omega_\perp = 2\pi \times 210$ Hz, our prediction is $\Omega_1 = 2\pi \times 147$ Hz, which coincides exactly which the experimental measures [7].

The fact that simple mean field theories are still valid when vortices enter into the dynamics, and that we may still expect quantitative predictions based on this simple models is interesting and has been shown in many other phenomena [6]. The striking result that the combined effect of asymmetry and nonlinearity may lead to the phenomenology here studied is another example of the richness of behaviors that one may expect from these nonlinear Quantum mesoscopic systems.

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